

Message

From: Volz, Stephanie [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=56ABDBFDC7CC496EA71C6AC9CE20C36C-SVOLZ]
Sent: 8/29/2019 1:30:48 PM
To: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
Subject: RE: PFAS Question

Nothing confidential. You're fine.

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Thursday, August 29, 2019 5:34 AM
To: Volz, Stephanie <Volz.Stephania@epa.gov>
Subject: RE: PFAS Question

Stephanie,

In looking up Lams contact info I inadvertently ccd him as I failed to remove him from the cc line. I am sorry about that. I hope not of this was confidential. I will try to recall the email if I can.

Mark

From: Volz, Stephanie <Volz.Stephania@epa.gov>
Sent: Wednesday, August 28, 2019 4:48 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: PFAS Question

Excellent. Thank you so much. It appears I have PFO5DoDA in my samples.

We would love to get our hands on some reference material. How can I make that happen? We're analyzing water samples for these compounds and I'm sure you know what other compounds are up and coming on the horizon (ADONA...).

Perfluoro-3,6-dioxo-4-methyl-7-octene-1-sulfonic acid	PFESA Byproduct 1*	29311-67-9	C ₇ H ₁₃ O ₅ S	443.93371
2-[1-[difluoro(1,2,2,2-tetrafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoroethanesulfonic acid	PFESA Byproduct 2*	749836-20-2	C ₇ H ₂ F ₁₄ O ₅ S	463.93994
2,2-difluoro-2-(trifluoromethoxy) acetic acid	PFMOAA*	674-13-5	C ₃ HF ₅ O ₃	179.98459
Perfluoro-3,5-dioxahexanoic acid	PFO2HxA*	39492-88-1	C ₄ HF ₇ O ₄	245.97631

Perfluoro-3,5,7-trioxaoctanoic acid	PFO3OA*	39492-89-2	C ₅ HF ₉ O ₅	311.96803
Perfluoro-3,5,7,9-tetraoxadecanoic acid	PFO4OA*	39492-90-5	C ₆ HF ₁₁ O ₆	377.95975
Perfluoro-3,5,7,9, 11-pentadoddecanoic acid	PFO5OA or TAFN4*	39492-91-6	C ₇ HF ₁₃ O ₇	443.95147
Propanoic Acid, 2,2,3,3-tetrafluoro-3-(trifluoromethoxy)-	PFECA F or PMPA*	377-73-1	C ₄ HF ₇ O ₃	229.98139

We were also trying to quantify N-MeFOSE and N-EtFOSE but were unable to recover the associated internal standards. We did additional washes of the SPE cartridge and now we're thinking they may have washed through during the column conditioning. We still need to test that theory out.

Thanks again,
Steph

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Wednesday, August 28, 2019 2:02 PM
To: Volz, Stephanie <Volz.Stephanie@epa.gov>
Subject: RE: PFAS Question

Stephanie,

First for the PFESA BP2, yes having two peaks is typical. Something about having asymmetric carbons or something like that. I don't recall the details. The peaks are usually exactly the same size, but for sure 2 peaks.

For the PFESA BP1 and the PFO5DoDA they are similar in molecular weight however two things will stand out.

1. The molecular weight between two compounds PFESA BP1 (442.9264) and PFO5DoDA (442.9442) is 40.2 ppm. Your QTOF should be able to tell them apart based on mass due to the EIC being extracted can be chosen to be 5 ppm or so.
2. The PFESA BP1 will have a sulfonate (m/z 79.9) and a FSO₃ (m/z 98.9) transition just like the PFOS, PFHxS and PFBS do.
3. PFO5DoDA will have a 84.9907 fragment however the PFESA BP1 will not. I have no idea what the 283.1367 fragment is. Also it will

Glad to chat if you need more later on tomorrow. Here is my 2015 paper in the SI that may have some details you can use. I also have standards for all of these I can share if you need them.

Mark

From: Volz, Stephanie <Volz.Stephanie@epa.gov>

Sent: Wednesday, August 28, 2019 3:06 PM

To: Strynar, Mark <Strynar.Mark@epa.gov>

Subject: PFAS Question

Mark,

I just left you a phone message but was wondering if you have any insight or documentation into telling these two compounds (PFESA Byproduct 1 and PFO5DA) apart. I don't have any reference material but I am working on a QTOF. I'm seeing 442.943 and 886.896 for the dimer. I'm seeing the peak at 8.175 minutes and fragments of 283.1367 and 84.9907. I don't have background data on retention time or fragments for either compound.

Compound Name	Formula	RT (min)	Mass	m/z	Adduct/dimer	Fragments	Fragments	Fragments	CAS	IUPAC N
---------------	---------	----------	------	-----	--------------	-----------	-----------	-----------	-----	---------

PFESA (Byproduct 1)	C7HF13O5S	443.93371	442.9441926	886.8596	(2M-H)-	?	?	?	29311-67-9	Perfluoro-3,
PFO5DA	C7HF13O7	443.95147	442.926434	886.8951	(2M-H)-	?	?	?	39492-91-6	Perfluoro-3,5

Also, I'm seeing a doublet for PFESA Byproduct 2 at 7.171 and 7.294 minutes. Do you know if that's typical?

Best Regards,

Stephanie Volz
US EPA/NEIC
1 Denver Federal Center, Bldg 25, Door E3
Denver, Colorado 80225
303-462-9127